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14. ABSTRACT

Quantum Monte Carlo simulations, supplemented by diagonalization, were used to see how efficiently a quantum computer could solve optimization problems using the quantum adiabatic algorithm (QAA). Comparisons were made with a classical heuristic algorithm, WalkSAT. A preliminary study was also made to see if the QAA could solve the graph isomorphism problem. Several optimization problems were considered. Those of the K-SAT type, which, in mean field theory have a "random first order transition" , were found to have an exponentially small

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Quantum Adiabatic Algorithm, Optimization, Monte Carlo, quantum computer, satisfiability problems, spin glass, quantum phase transition

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Peter Young
UU	UU	UU	UU		19b. TELEPHONE NUMBER
					831-459-4151

Report Title

Final Report

ABSTRACT

Quantum Monte Carlo simulations, supplemented by diagonalization, were used to see how efficiently a quantum computer could solve optimization problems using the quantum adiabatic algorithm (QAA). Comparisons were made with a classical heuristic algorithm, WalkSAT. A preliminary study was also made to see if the QAA could solve the graph isomorphism problem. Several optimization problems were considered. Those of the K-SAT type, which, in mean field theory have a "random first order transition" , were found to have an exponentially small energy gap at the quantum phase transition. We also studied a spin glass problem in which the gap was found to be exponentially small not at the phase transition but beyond it in the "quantum spin glass" phase. These results show that that the simplest implementation of the QAA would require an amount of computer time which increases exponentially with problem size. For the future, it would be useful to test whether better results could be obtained by considering cleverer paths in "Hamiltonian space", and by considering different types of problem where the absolute ground state is not needed, only a good approximation to it.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
12/06/2012	4.00	Itay Hen, A. Young. Solving the graph-isomorphism problem with a quantum annealer, Physical Review A, (10 2012): 0. doi: 10.1103/PhysRevA.86.042310
12/06/2012	2.00	A. P. Young, V. N. Smelyanskiy. First-Order Phase Transition in the Quantum Adiabatic Algorithm, Physical Review Letters, (01 2010): 0. doi: 10.1103/PhysRevLett.104.020502
12/06/2012	3.00	A. P. Young, Itay Hen. Exponential complexity of the quantum adiabatic algorithm for certain satisfiability problems, Physical Review E, (12 2011): 0. doi: 10.1103/PhysRevE.84.061152
12/06/2012	5.00	Edward Farhi, David Gosset, Itay Hen, A. Sandvik, Peter Shor, A. Young, Francesco Zamponi. Performance of the quantum adiabatic algorithm on random instances of two optimization problems on regular hypergraphs, Physical Review A, (11 2012): 0. doi: 10.1103/PhysRevA.86.052334
TOTAL:	**4**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Colloquium on ``Complexity of the Quantum Adiabatic Algorithm'', Princeton, September 24, 2009.

Invited lecture on ``Complexity of the Quantum Adiabatic Algorithm'' at Winter School on Quantum Information Science at Natl.~Cheng Kung Univ., Tainin, Taiwan, December 19--22, 2009

Talk on ``First order phase transitions in the Quantum Adiabatic Algorithm'' at the March meeting of the APS, March 15--19, 2010.

Invited talk on ``First order phase transition in the Quantum Adiabatic Algorithm'', at the Conference on Quantum Statistical Mechanics, Computation, and Information, ICTP, Trieste, June 14-18, 2010

Talk on ``First order phase transition in the Quantum Adiabatic Algorithm'', at Statphys24, Cairns, Australia, July 19-23.

Invited talk on "Efficiency of the Quantum Adiabatic Algorithm" at the third international workshop on dynamics and manipulation of quantum systems (DMQS2010), Tokyo, February 14--16, 2011.

Invited talk on "Quantum Adiabatic Algorithms" at Summer School on "Quantum Information meets Statistical Mechanics" at El Escorial, Spain, July 11--15, 2011.

Invited talk on "Quantum adiabatic algorithms" at the International Workshop on Simulation and Manipulation of Quantum Systems for Information Processing (SMQS-IP2011), J\"ulich Supercomputing Centre, Germany, October 17--19, 2011.

Invited talk on ``Mind the gap, solving optimization problems with a quantum computer'', NASA Quantum Future Technologies Conference, NASA Ames, January 18, 2012.

Number of Presentations: 9.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<div align="center">

Peer-Reviewed Conference Proceeding publications (other than abstracts):

</div>

Received | Paper

12/06/2012   6.00   A.P. Young, S. Knysh, V.N. Smelyanskiy. The complexity of the Quantum Adiabatic Algorithm,
Conference on Computational Physics Kaohsiung, Taiwan, . , . : ,

TOTAL: **1**

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

<div align="center">

(d) Manuscripts

</div>

Received | Paper

TOTAL:

Number of Manuscripts:

<div align="center">

Books

</div>

Received | Paper

TOTAL:

<div align="center">

Patents Submitted

</div>

<div align="center">

Patents Awarded

</div>

<div align="center">

Awards

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Awarded the Humboldt Prize (Humboldt Research Award) in 2011.

Elected member of the American Academy of Arts and Sciences in 2012

Awarded the 2009 Aneesur Rahman Prize for Computational Physics from the American Physical Society.

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Itay Hen	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
A. P. Young	0.22	
FTE Equivalent:	**0.22**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics
This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:······ 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:······ 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale): 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering: 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME	
Total Number:	

Names of personnel receiving PHDs

NAME	
Total Number:	

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Technology Transfer

<p style="text-align:center">Agreement Number: W911NF0910391
"Determining the Complexity of the Quantum Adiabatic
Algorithm using Quantum Monte Carlo simulations"
Principal Investigator: A. Peter Young</p>

1   Introduction

This project is to study whether an eventual quantum computer could solve optimization problems more efficiently than a classical computer using the "quantum adiabatic algorithm" (QAA) described below.

The grant has led to six publications [1, 2, 3, 4, 5, 6], one of which [2] is a conference presentation. In addition, the PI presented results at nine international conferences which did not have proceedings. Both the PI and post-doc gave additional seminars on the research.

The initial work was done in collaboration with Smelyanskiy and Sergey Knysh, and a visiting student, Marco Guidetti participated in one of the papers, Ref. [3]. The work for the last paper [6] started during fall 2010 when the PI was on sabbatical at MIT in the group of Eddie Farhi (whose group invented the QAA in 2001). This paper [6] involved a collaboration of Farhi, his student David Gosset, Peter Shor (also at MIT), Francesco Zamponi from Paris, and Anders Sandvik from Boston University, in addition to the PI and post-doc.

Since the detailed results are in the papers, it does not seem to be necessary to repeat them all here. Rather I will give a general introduction followed by comments on the work in each of the papers. Naturally the papers also include a much larger bibliography.

For some *specialized* problems, such as factoring large integers, which is relevant for cryptography, a quantum computer is *known* to be much more efficient than a classical computer [7, 8]. The present project investigated whether, in addition, a quantum computer could solve a *wide range* of hard "optimization" problems more efficiently than a classical computer using the quantum adiabatic algorithm (QAA) [9]. The main technique used was Quantum Monte Carlo (QMC) simulations, which both the PI and the post-doc are very familiar with. Exact diagonalization was also used in some of the work. In addition, a comparison was made between the results from the QAA and a *classical* heuristic algorithm called WalkSAT.

In the QAA, a quantum Hamiltonian is realized by the connections in a quantum computer. A time-dependent control parameter, $s(t), (0 \leq s(t) \leq 1)$, is smoothly varied, taking the system from a "driver Hamiltonian" $\mathcal{H}_\mathrm{D}$, which is easy to solve, at $t = 0$ $(s(0) = 0)$, to the non-trivial "problem Hamiltonian" of interest $\mathcal{H}_\mathrm{P}$ at time $\mathcal{T}$ $(s(\mathcal{T}) = 1)$. The total Hamiltonian is therefore

$$\mathcal{H}(t) = [1 - s(t)]\mathcal{H}_\mathrm{D} + s(t)\mathcal{H}_\mathrm{P}. \tag{1}$$

For $\mathcal{H}_\mathrm{P}$ we consider binary optimization problems expressed in terms of classical bits $z_i = (0, 1)$, which we represent by Ising spins taking values $\sigma_i^z = 1 - 2z_i = (1, -1)$. The simplest driver Hamiltonian is then

$$\mathcal{H}_\mathrm{D} = -h \sum_{i=1}^{N} \sigma_i^x, \tag{2}$$

where σ_i^x is the x-component Pauli matrix and h is a "transverse field".

<div style="text-align:center">1</div>

The quantum computer is started in the (trivial) ground state of the driver Hamiltonian and, if the process is slow enough to be adiabatic, it ends up in the ground state of the problem Hamiltonian, which solves the problem. The time taken to do this, $\mathcal{T}$, is called the complexity. Since the process is slow and smooth, it is easier to screen out noise, which would destroy quantum coherence, in the QAA than in other quantum algorithms, which proceed by a series of *discrete* unitary transformations. Hence there is a substantial experimental effort to build a quantum computer to implement the QAA. In particular, D-Wave has built a quantum annealer with over 100 qubits to implement the QAA. One of these will be installed at NASA-Ames, with financial support from Google. The PI on supported by the grant, Itay Hen, now at NASA-Ames, will provide theoretical support for this project.

An important class of optimization problems is that known as "NP-hard" [10], since their complexity is found to grow exponentially with problem size N, and, furthermore, any problem in a wide set, call "NP", can be mapped into an NP-hard problem in polynomial time.

A bottleneck will be where the gap between the ground state and the first excited state becomes very small, since the time needed to maintain adiabatic evolution is proportional to the square of the inverse of the minimum gap. The QMC simulations compute the gap as a function of the control parameter s for each instance, locate its minimum value, and see how the minimum gap, averaged in some suitable way, varies with system size.

The funding was mainly used to support a full-time post-doc, Itay Hen. Some funding was also used for summer salary for the PI, and for travel to conferences. In the first year, some computers were bought to increase the computer power available for the project. The post-doc is continuing to work on related problems as a staff scientist at NASA Ames under the supervision of Vadim Smelyanskiy.

1.1   Reference [1]

This paper, in collaboration with Vadim Smelyanskiy and Sergey Knysh, studied a particular constraint satisfaction problem called exact cover using quantum Monte Carlo simulations. It was found that, as the size increases, there is a first order (i.e. discontinuous) quantum phase transition during the evolution of the QAA for instances of size greater than about 100. A first order transition leads to a minimum energy gap which decreases exponentially with problem size, and hence to an exponentially large time for the QAA to solve the problem.

1.2   Reference [2]

This is a paper presented at the Conference on Computational Physics 2009 (CCP2009) in Kaoshing, Taiwan. CCP2009 is part of the series of conferences organized by the computational divisions of American Physical Society and the European Physical Society on Physics Computing. This conference write up is short, because of page limitations, and is a summary of Ref. [1].

1.3   Reference [3]

This paper was in collaboration with a visiting student, Marco Guidetti. It studied the complexity of four constraint satisfaction problems using a classical, heuristic algorithm

called WalkSAT. The aim of this study was to get results from a classical algorithm with a view to eventually comparing them with those from the quantum adiabatic algorithm. This latter stage was done in Ref. [4].

Three of the four models are in the NP-hard complexity class, and one, called 3-XORSAT, is in the P complexity class for which there exists a polynomial time algorithm. All show exponential complexity for large sizes. Curiously, the hardest problem for WalkSAT is 3-XORSAT, the one in P. Although it is not surprising that WalkSAT does not solve the this problem in polynomial time, since the polynomial time algorithm is special, and is completely unrelated to the stochastic methods in WalkSAT, it is, nonetheless, quite striking that it is actually *harder* for WalkSAT than the problems in NP. The strange result that 3-XORSAT is very "glassy" (i.e. very hard to solve by general purpose algorithms) while being easy to solve by a special algorithm, has been discussed recently to illustrate problems in a claimed proof by Deolalikar that P is not equal to NP, one of the major unsolved problems in mathematics. See for example the discussion in Refs. [11, 12].

1.4   Reference [4]

This paper determined the complexity of several constraint satisfaction problems using the quantum adiabatic algorithm in its simplest implementation. This was done, by studying the size dependence of the gap to the first excited state of "typical" instances using QMC simulations. The result is that, at large sizes N, the complexity increases exponentially for all models that was studied. A comparison was made with the the complexity obtained from the analogous classical algorithm WalkSAT which was found in Ref. [3]. It was seen that the harder the problem is for the classical algorithm, the harder it is also for the quantum adiabatic algorithm.

This work was selected by the American Physical Society for presentation on their web site which spotlights exceptional research:
`http://physics.aps.org/synopsis-for/10.1103/PhysRevE.84.061152`.

1.5   Reference [5]

This paper proposed a method using a quantum annealer, an analog quantum computer based on the principles of quantum adiabatic evolution, to solve the graph isomorphism problem, in which one has to determine whether two graphs are isomorphic (i.e., can be transformed into each other simply by a relabeling of the vertices). The paper demonstrated the capabilities of the method by focusing on graphs with particularly high symmetry called strongly regular graphs, though some other graphs were studied as well. This was a preliminary study so only quite small graphs were considered which could be treated by diagonalization or a related method. In future work, it would be interesting to study larger sizes using Quantum Monte Carlo simulations. The paper also showed that the method is applicable, within certain limitations, to currently available quantum hardware such as D-Wave One.

1.6   Reference [6]

This paper was a collaboration of the PI and post-doc with Eddie Farhi, David Gosset, Peter Shor, Francesco Zamponi and Anders Sandvik. In it we studied the performance of

the quantum adiabatic algorithm on random instances of two combinatorial optimization problems, 3-regular 3-XORSAT and 3-regular max-cut (a spin glass problem). We used quantum Monte Carlo and quantum cavity methods. Using these techniques we find that the quantum adiabatic algorithm fails to solve either of these problems efficiently. For the 3-XORSAT problem it fails *at* the quantum phase transition where the energy gap has a minimum which is exponentially small in the problem size N. For the spin glass problem it fails *beyond* the quantum phase transition, i.e. in the quantum spin glass phase, where, again, the minimum gap decreases exponentially with N.

2 Possible future work

The work supported by the grant showed that the *simplest implementation* of the QAA does not seem to be more efficient for solving some classes of optimization problems than a classical algorithm. However, there is a lot of flexibility in the method. To implement the QAA one has to decide on a "path in Hamiltonian space", starting with a simple Hamiltonian for which the system can be prepared in the ground state, and ending with the specified problem Hamiltonian. The present work just took the simplest path, in which the driver Hamiltonian, $\mathcal{H}_D$, is a sum of transverse fields, the same on all sites, and the the total Hamiltonian is a linear combination of $\mathcal{H}_D$ and the problem Hamiltonian. In future work it would be desirable to find a more clever path in Hamiltonian space to increase the value of the minimum gap. Some ideas for that, for a problem not studied by the PI, have been proposed in Ref. [13].

It would also be useful to develop further the possible application of quantum annealing (QAA) to solve the graph isomorphism problem beyond the preliminary study in Ref. [5]. The graph isomorphism problem is interesting because, like integer factoring, it is a problem for which there is no known classical polynomial-time classical algorithm, and yet it is probably not in the NP-hard category. Since a quantum polynomial-time algorithm has been found [7] for integer factoring, it is worth investigating whether the same can be done for another problem in this category, which is intermediate between P and NP-hard, namely graph isomorphism.

In all problems discussed so far in this report, the goal has been to study the exact ground state. For many problems of practical importance, it is not necessary to find the state of lowest energy; rather, any state with energy close to that of the ground state will do. For some problems, even finding an energy close to the ground state is hard [14]. It would be worthwhile to see if the QAA could find a close-by energy more efficiently than a classical algorithm.

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